

WHAT IS CLAIMED IS:

1. A computer implemented method for modifying an experimental electron density map comprising the steps of:

providing a set of selected known experimental and model electron density maps;

5 creating standard templates of electron density from the selected experimental and model electron density maps by clustering and averaging values of electron density in a spherical region about each point in a grid that defines each selected known experimental and model electron density maps;

creating histograms from the selected experimental and model electron  
10 density maps that relate the value of electron density at the center of each of the spherical regions to a correlation coefficient of a density surrounding each corresponding grid point in each one of the standard templates;

applying the standard templates and the histograms to grid points on the experimental electron density map to form new estimates of electron density at  
15 each grid point in the experimental electron density map.

2. The method of Claim 1, wherein the steps of creating standard templates and creating histograms include the step of excluding electron density information from each grid point as clustering and averaging values are generated for that grid point and as histograms are generated for that grid point.

3. The method of Claim 1, wherein the step of creating standard templates further includes the steps of:

generating three separate sets of templates corresponding to grid points that have either low, medium, or high electron density;

5 selecting a subset of templates from the three sets of templates that have a low mutual correlation; and

selecting a final set of templates from the subset of templates that are selected to maximize the predictive power of the final set of templates.

4. The method of Claim 1, where the step of creating histograms includes the steps of:

comparing the electron density value at each grid point in each of the templates with the electron density value at corresponding grid points in a set of  
5 high quality electron density maps and determine a correlation coefficient at each grid point;

identifying two templates that have the highest and next-highest correlation coefficients; and

10 tabulating the value of the electron densities in the two templates and normalize to yield an estimate of the probability distribution of an electron density at each grid point.

5. The method of Claim 2, wherein the step of creating standard templates further includes the steps of:

generating three separate sets of templates corresponding to grid points that have either low, medium, or high electron density;

5 selecting a subset of templates from the three sets of templates that have a low mutual correlation; and

selecting a final set of templates from the subset of templates that are selected to maximize the predictive power of the final set of templates.

6. The method of Claim 2, where the step of creating histograms includes the steps of:

comparing the electron density value at each grid point in each of the templates with the electron density value at corresponding grid points in a set of  
5 high quality electron density maps and determine a correlation coefficient at each grid point;

identifying two templates that have the highest and next-highest correlation coefficients; and

10 tabulating the value of the electron densities in the two templates and normalize to yield an estimate of the probability distribution of an electron density at each grid point.